

Ethyl 1-thio-beta-D-galactopyranoside
56245-60-4 | DTXSID70440378

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 4.08e-02 mol/L

Global applicability domain: Inside

Local applicability domain index: 4.61e-01

Confidence level: 7.77e-01

Nearest Neighbors from the Training Set

Image not found

Chlorendic acid

Measured: 9.00e-03

Predicted: 1.07e-02

Image not found

2-(carboxymethylsulfanylcarbothioylamino)acetic acid

Measured: 5.00e-02

Predicted: 5.38e-02